(91) Expressions for Fermi energy μ.

(i) At $T = 0$

N particles in volume V

Number particles with $\epsilon \to \epsilon + d\epsilon$	$=$	Number states $\epsilon \to \epsilon + d\epsilon$	$\times$	Prob of state occupation

$$n(\epsilon)\, d\epsilon = g(\epsilon)\, d\epsilon \times f(\epsilon)$$

$$N = \int_0^\infty n(\epsilon)\, d\epsilon = \int_0^\infty g(\epsilon)\, d\epsilon \times f(\epsilon)$$

Recall $g(\epsilon)\, d\epsilon = 4\pi V \left(\frac{2m}{h^2}\right)^{3/2} \epsilon^{1/2}\, d\epsilon$

$$N = \int_0^\infty 4\pi V \left(\frac{2m}{h^2}\right)^{3/2} \epsilon^{1/2}\, d\epsilon \,.\, f(\epsilon)$$

but $f(\epsilon) = 1 \qquad \epsilon < \mu$

$f(\epsilon) = 0 \qquad \epsilon > \mu$

Thus

$$N = 4\pi V \left(\frac{2m}{h^2}\right)^{3/2} \int_0^\mu \epsilon^{1/2}\, d\epsilon$$

gives $N = 4\pi V \left(\frac{2m}{h^2} \right)^{3/2} \cdot \frac{2}{3} \mu^{3/2}$

$$\mu = \left(\frac{\hbar^2}{2m} \right) \left(3\pi^2 \frac{N}{V} \right)^{2/3}$$

Strictly this μ should be denoted $\mu(0)$ $\leftarrow$ evaluated at $T = 0$.

Alternative method for $\mu(0)$.

Recall k space spanned by quantum states with $k_x = \frac{2\pi}{L} \cdot n_x$, $k_y = \frac{2\pi}{L} n_y$ ..

and particle kinetic energy ϵ given by

$$\epsilon = \frac{\hbar^2 k^2}{2m}$$

Corresponding to Fermi energy μ is k_F

where $\mu = \frac{\hbar^2 k_F^2}{2m}$

where $k < k_F$ states filled

$k > k_F$ states empty

Then

$$N = \text{number of filled states}$$

$$N = \underbrace{2}_{\uparrow \text{ and } \downarrow} \times \underbrace{\frac{4}{3}\pi k_F^3}_{\text{volume of } k \text{ space}} \times \underbrace{\frac{1}{(2\pi/L)^3}}_{\text{volume of } k \text{ space per state.}}$$

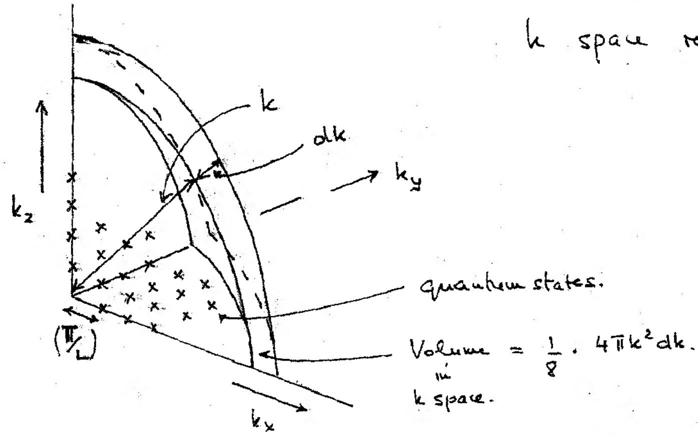
$$N = \frac{8\pi}{3} k_F^3 \cdot \frac{V}{(2\pi)^3}$$

$$k_F^3 = \frac{3\pi^2 N}{V}$$

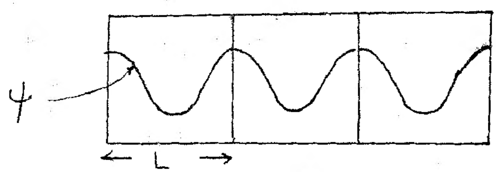
$$\mu(0) = \frac{\hbar^2 k_F^2}{2m} = \left(\frac{\hbar^2}{2m}\right)\left(\frac{3\pi^2 N}{V}\right)^{2/3}$$

Standing wave boundary conditions.

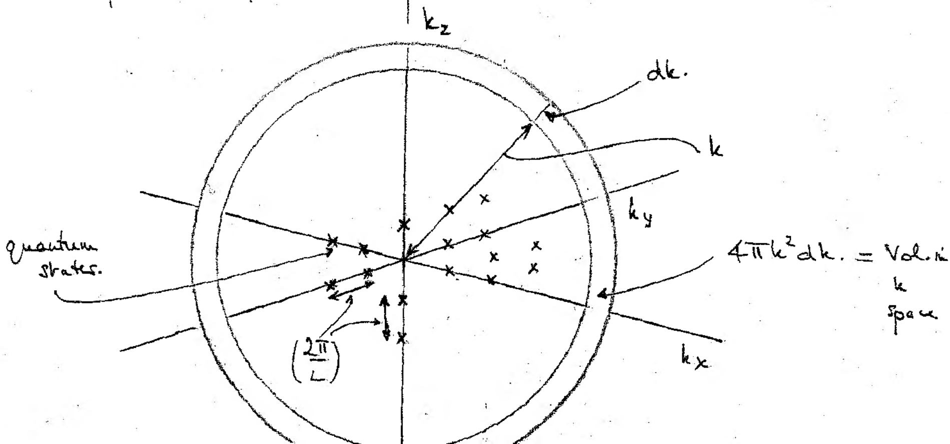
k space representation.



Periodic Boundary conditions.



k space representation



Classical and quantum limits.

Combining $$A = \frac{N}{V}\left(\frac{h^2}{2\pi m k T}\right)^{3/2}$$

and $$\mu(0) = \left(\frac{\hbar^2}{2m}\right)\left(3\pi^2\frac{N}{V}\right)^{2/3} = kT_F$$

get $$A = \frac{8}{3\sqrt{\pi}}\left(\frac{T_F}{T}\right)^{3/2}$$

Classical condition

$A \ll 1$ equivalent to $T \gg T_F$

Quantum condition

$A \gg 1$ equivalent to $T \ll T_F$

Where are actual systems on this scale?

1. Conduction electrons in copper.

For Cu $\frac{N}{V} = 8.5 \times 10^{28}\ m^{-3}$

95

$$kT_F = \left(\frac{\hbar^2}{2m}\right)\left(3\pi^2\frac{N}{V}\right)^{2/3}$$

gives $T_F \simeq 10^5$ K

Lab measurements taken with $T \ll T_F$

Conduction electrons at quantum limit of F-D gas

2. He^3 — gas – classical
— liquid – quantum

in low temp section

3. Neutron stars

Large densities $\frac{N}{V}$ give $T_F \simeq 10^{10}$ K

Actual temperature $T \sim 10^7$ K

Neutron gas in star at quantum limit.

Variation of Fermi energy μ with temperature T.

Q. Does μ vary with T ?

A. Yes – but in quantum (degenerate) limit – the variation is small.

Analysis.

Recall $$N = \int_0^\infty g(\epsilon).\, f(\epsilon)\, d\epsilon$$

Procedure – do this integration (i) at $T = 0$

(ii) at $T > 0$

and equate.

Write $g(\epsilon) = C\epsilon^{1/2}$ where $C = 4\pi V\left(\frac{2m}{h^2}\right)^{3/2}$

(i) At $T = 0$

$$N = \int_0^\infty C\epsilon^{1/2} f(\epsilon)\, d\epsilon = \int_0^{\mu(0)} C\epsilon^{1/2}\, d\epsilon = \frac{2}{3} C[\mu(0)]^{3/2}$$

(ii) At $T > 0$

$$N = \int_0^\infty C\epsilon^{1/2} f(\epsilon)\, d\epsilon$$

To do this integral use method of Guenault Appendix 3.

Write integral in form $$N = \int_0^\infty \left(\frac{dF}{d\epsilon}\right) f(\epsilon)\, d\epsilon$$

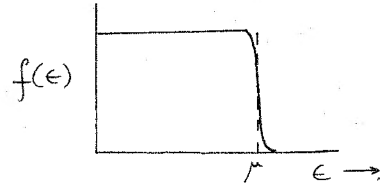
$$= \left[F(\epsilon) f(\epsilon)\right]_0^\infty - \int_0^\infty F(\epsilon)\left(\frac{df}{d\epsilon}\right) d\epsilon$$

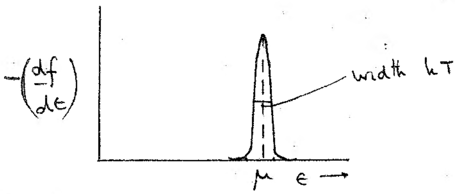
In our case $\left(\frac{dF}{d\epsilon}\right) = C\epsilon^{1/2}$

$$F(\epsilon) = \frac{2}{3} C \epsilon^{3/2}$$

Then $$N = \left[\frac{2}{3} C \epsilon^{3/2} f(\epsilon) \right]_0^\infty - \int_0^\infty \frac{2}{3} C \epsilon^{3/2} \left(\frac{df}{d\epsilon}\right) d\epsilon$$

$$N = 0 - \int_0^\infty \frac{2}{3} C \epsilon^{3/2} \left(\frac{df}{d\epsilon}\right) d\epsilon$$





See from graphs that integrating with $-\left(\frac{df}{d\epsilon}\right)$ picks out $\frac{2}{3} C \epsilon^{3/2}$ at $\epsilon = \mu$. — due to finite width kT — there is correction term.

Guenault Appendix 3

Gives

$$N = \frac{2}{3} C \mu^{3/2} + \frac{\pi^2}{6} (kT)^2 \left(\frac{d^2F}{d\epsilon^2}\right)_{\epsilon=\mu}$$

Thus $$N = \frac{2}{3} C \mu^{3/2} + \frac{\pi^2}{6} . (kT)^2 . \frac{1}{2} \frac{C}{\mu^{1/2}}$$

Equate $T=0$ and $T \neq 0$ integrals for N

$$\frac{2}{3} C \mu(0)^{3/2} = \frac{2}{3} C \mu^{3/2} + \frac{\pi^2}{12} (kT)^2 \frac{C}{\mu^{1/2}}$$

$$\mu(0)^{3/2} = \mu^{3/2} \left[1 + \frac{3}{2} \cdot \frac{\pi^2}{12} \cdot \frac{(kT)^2}{\mu^2} \right]$$

$$\mu = \mu(0) \left[1 + \frac{3}{2} \cdot \frac{\pi^2}{12} \cdot \left(\frac{kT}{\mu}\right)^2 \right]^{-2/3}$$

Small since $kT \ll \mu$

$$\mu = \mu(0) \left[1 - \frac{\pi^2}{12} \left(\frac{kT}{\mu}\right)^2 + \dots \right]$$

Small variation of μ with T ...

Variation of Fermi energy μ with temperature T see sheets.

Thermodynamic quantities.

Energy U

$$U = \sum_i n_i \epsilon_i$$

In gas $U = \int_0^\infty \epsilon \, g(\epsilon) \, f(\epsilon) \, d\epsilon$

At $T=0$

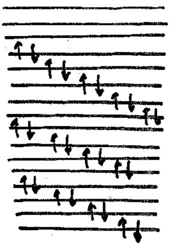
$$U(0) = \int_0^{\mu(0)} \epsilon \, . \, C \epsilon^{1/2} \, d\epsilon = \int_0^{\mu} C \epsilon^{3/2} \, d\epsilon$$

$$U(0) = \frac{2}{5} C \mu^{5/2}$$

But above $N = \frac{2}{3} C \mu^{3/2}$

Thus $U(0) = \frac{3}{5} N \mu .$

$U(0) = \frac{3}{5} N\mu$ is very large zero point energy — because of Pauli principle not allowing more than ↑ and ↓ fermions in same state.



← μ

— fermions cannot all go to lowest states.

For $T > 0$ but $T \ll T_F$

$$U = \int_0^\infty \epsilon \,.\, C\epsilon^{1/2} f(\epsilon)\, d\epsilon$$

Similar integration to that for Fermi energy gives

$$U = U(0) + U(\text{thermal})$$

$$U = \frac{3}{5} N\mu + \frac{\pi^2}{6} (kT)^2 g(\mu)$$

Zero point energy

Thermal energy

$g(\mu)$ = density of states at Fermi energy

Density of states at fermi energy – see diagram on sheet.

Understand form of U (thermal) from

(i) Only states that can be excited at temp T lie within energy kT of μ

(ii) Number of particles involved $= g(\mu) . kT$

Excitation energy / particle $= kT$

Thermal excitation energy $U(th) \simeq (kT)^2 g(\mu)$

Graph of U vs T – see sheet.

For $T \gg T_F$

Classical limit.

$$U \rightarrow \frac{3}{2} NkT.$$

59

Heat capacity C_v

$$C_v = \left(\frac{\partial U}{\partial T}\right)_V = \frac{\partial}{\partial T}\left[\frac{3}{5}N\mu + \frac{\pi^2}{6}(kT)^2 g(\mu)\right]$$

$$C_V = \frac{\pi^2}{3} k^2 T \, g(\mu)$$

Graph of C_v vs T — see sheet

Points

1. As $T \to 0$ $C_v \to 0$

2. In expt'l range for conduction electrons

   C_V is (i) small

   (ii) $\propto$ temperature T.

3. For $T \gg T_F$ — classical limit

$$C_V = \frac{\partial U}{\partial T} \longrightarrow \frac{\partial}{\partial T}\left(\tfrac{3}{2}NkT\right) = \frac{3}{2}Nk.$$

4. For $g(\epsilon) = C\epsilon^{1/2}$ — see diagram

$$g(\mu) = \frac{3N}{}$$

Then in quantum region can write

$$C_V = \frac{\pi^2}{3} k^2 T \; g(\mu) = \frac{\pi^2}{3} . k^2 T . \frac{3N}{2\mu}$$

$$C_V = \frac{\pi^2}{3} \left(\tfrac{3}{2} N k \right) . \left(\frac{kT}{\mu} \right)$$

classical x fermi function (small).

Pressure P.

First Law $\quad dU = TdS - pdV$

For constant S $\quad p = -\left(\frac{\partial U}{\partial V}\right)_S$

Quantum limit

$$U = \sum_i n_i \epsilon_i$$

$$P = -\left(\frac{\partial U}{\partial V}\right)_S = -\sum_i n_i \left(\frac{\partial \epsilon}{\partial V}\right)$$

n_i const at const S

Recall $$\epsilon = \frac{\hbar^2 k^2}{2m}$$

$$k = \frac{2\pi n}{L}$$

$$k^2 \propto L^{-2} \quad \text{or} \quad V^{-2/3}$$

Thus $$\epsilon \propto V^{-2/3} = K V^{-2/3}$$

Hence $$\left(\frac{\partial \epsilon}{\partial V}\right) = -\frac{2}{3} K V^{-5/3} \equiv -\frac{2}{3}\frac{\epsilon}{V}$$

Then $$p = -\sum \left(-\tfrac{2}{3}\right) \frac{n_i \epsilon_i}{V}$$

$$p = \frac{2}{3}\frac{U}{V}$$

Points

1. This large pressure at quantum limit due to large $U(0)$ – keeps neutron stars stable against gravitational force

2. At classical limit $T \gg T_F$

$$p \rightarrow \frac{NkT}{V}$$ — see sheet.

Entropy S.

Tedious to calculate

Know that as $T \rightarrow 0$
$S \rightarrow 0$

with particles condensing into lowest set of 'tower block' states.

Conduction electrons.

All exptl data occur in range $T \ll T_F$

Thus predicted properties in quantum limit of graphs of $\left.\begin{matrix} U \\ C_V \\ p \end{matrix}\right\}$ versus T.

103

Magnetisation of conduction electrons.

— see sheet.

Magnetisation M of conduction electrons.

M is magnetic moment $/m^3$ developed by conduction electrons when magnetic field B is applied to the piece of metal.

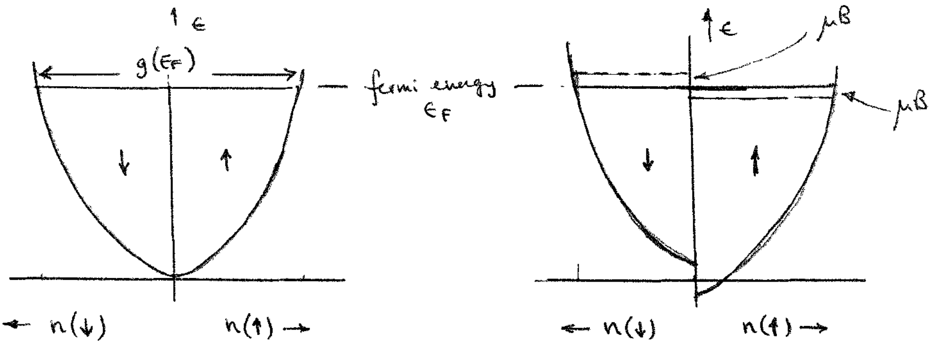
In field B each spin ½ electron has to orient spin

either parallel to B magnetic energy $= -\mu B$

or opposite to B magnetic energy $= +\mu B$

where μ = magnetic moment of electron (1 Bohr magneton)

Electron states. – use ϵ_F as fermi energy.



Zero field. Field B ↑

Magnetic moment $M = [n(\uparrow) - n(\downarrow)]\,\mu.$

When field B applied $\frac{1}{2}\,g(\epsilon_F).\mu B$ electrons

Then $M = \frac{1}{2} g(\epsilon_F) \mu B . 2\mu^*$

For $g(\epsilon_F) = \frac{3N}{2\epsilon_F}$

$$M = \frac{3N\mu^2 B}{2\epsilon_F} .$$

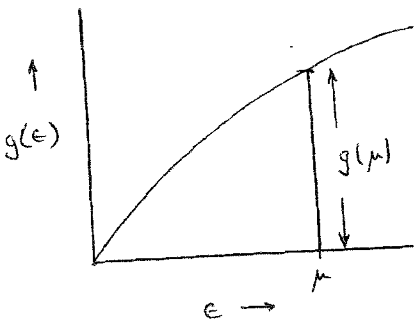
Predicts

1. Magnetic susceptibility $\chi = \frac{\mu_0 M}{B}$ is independent of temperature.

2. $\chi \propto$ density of states at fermi energy.

These confirmed by expt.

Density of states at the Fermi energy $g(\mu)$



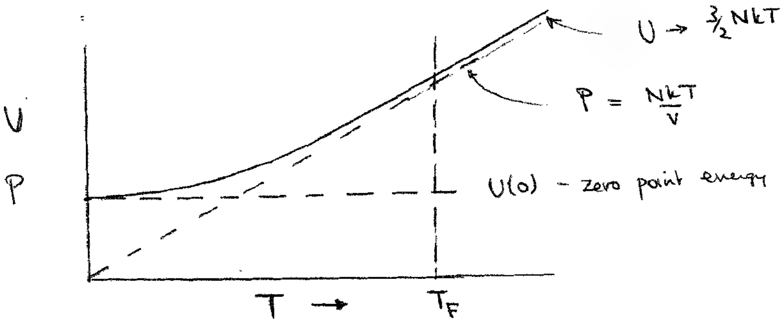
For $g(\epsilon) = C\epsilon^{1/2}$

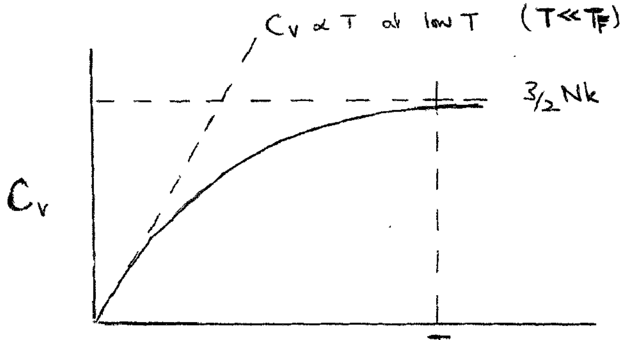
$$N = \frac{2}{3} C \mu^{3/2} \quad (T=0)$$

Then $g(\mu) = C\mu^{1/2} = \dfrac{3N}{2\mu}$.

Energy U versus T

Pressure P versus T





Statistical Mechanics Theory

N identical particles
Volume V
Thermal equilibrium at temperature T
Weak interactions

Particles distinguishable by position in solid

$$n_j = \frac{N}{Z} \exp\left(-\epsilon_j/kT\right)$$

$$Z = \sum_j \exp\left(-\epsilon_j/kT\right)$$

basic theory

Excitations in localised atoms

Gas particles in macroscopic box.
Particles indistinguishable

occupation number $f \gtrsim 1$

Quantum region
Behaviour depends whether $\psi(1,2)$ symmetric or antisymm under particle exchange

$\psi(1,2)$ antisymm

Fermi Dirac statistics

$$f(\epsilon) = \frac{1}{\exp(\epsilon-\mu/kT)+1}$$

μ = fermi energy

basic theory

Conduction electrons
Liquid He^3
He^3/He^4 liquid mixtures

$\psi(1,2)$ symmetric

Bose-Einstein statistics

$$f(\epsilon) = \frac{1}{B\exp(\epsilon/kT)-1}$$

basic theory

Radiation in enclosure
Phonons in solids
Superconductors
Liquid He^4

occupation number $f \ll 1$

Classical region
Maxwell Boltzmann statistics

$$f(\epsilon) = \frac{N}{Z}\exp(-\epsilon/kT)$$

$$Z = V\left(\frac{2\pi mkT}{h^2}\right)^{3/2}$$

basic theory

normal gases

Boson gases.

At low temperature

- fermions show "tower block" occupancy of energy states because of Pauli principle.

- bosons not subject to Pauli principle can show heavy population – "condensation into" the ground state.

  Can cause dramatic macroscopic effects.

Bose Einstein distribution

$$f(\epsilon) = \frac{1}{B\exp(\epsilon/kT) - 1}$$

Parameter B determined from

$$\sum_i n_i = N$$

Range of values of B.

$f(\epsilon)$ cannot be negative

As $\epsilon \to 0$ giving $\exp(\epsilon/kT) \to 1$

Sets range $1 < B$

(i) For conditions where $B \gg 1$ have

Classical region

B - Einstein distrib^n $\longrightarrow$ Maxwell Boltzmann

$$\frac{1}{B\exp(\epsilon/kT) - 1} \longrightarrow A\exp(-\epsilon/kT)$$

(ii) For $B \to 1$

Achieved at low temperature

Quantum region

In theory above - have determined B from

$$N = \sum_i n_i = \int_0^\infty g(k)\, f(k)\, dk \quad \text{or} \int_0^\infty g(\epsilon) f(\epsilon)\, d\epsilon$$

Boson case

$$N = \int_0^\infty g(k)\,dk\, f(k)$$

$$= \int_0^\infty \frac{4\pi V\, k^2 dk}{(2\pi)^3} \cdot \frac{1}{\left[B \exp\left(\frac{\hbar^2 k^2}{2mkT}\right) - 1 \right]}$$

$$\text{where} \quad \epsilon = \frac{\hbar^2 k^2}{2m}$$

$$\text{Putting} \quad y^2 = \frac{\hbar^2 k^2}{2mkT}$$

$$y\,dy = \frac{\hbar^2}{2mkT} \cdot k\,dk$$

$$y^2\,dy = \left(\frac{\hbar^2}{2mkT}\right)^{3/2} k^2\,dk$$

$$N = \frac{4\pi V}{(2\pi)^3} \left(\frac{2mkT}{\hbar^2}\right)^{3/2} \int_0^\infty \frac{y^2\,dy}{\left[B \exp(y^2) - 1\right]}$$

$$N = \frac{4}{\sqrt{\pi}} \cdot \underbrace{V \left(\frac{2\pi mkT}{h^2}\right)^{3/2}}_{Z \,\equiv\, \text{partition } f^n.} \int_0^\infty \frac{y^2\,dy}{\left[B \exp(y^2) - 1\right]}$$

Thus.

$$N = Z\,F(B)$$

where $$F(B) = \frac{4}{\sqrt{\pi}} \int_0^\infty \frac{y^2\,dy}{B\exp(y^2) - 1}$$

Graph of $F(B)$ vs B — see sheet.

Previously have defined degeneracy parameter

A where

$$A = \frac{N}{Z} = \left(\frac{N}{V}\right)\left(\frac{h^2}{2\pi mkT}\right)^{3/2}$$

Find

$A \ll 1$ classical region

$A \lessapprox 1$ changeover

$A > 1$ quantum region

Since both $= N/Z$

$$A = F(B)$$

Problems for theory.

Values of T, $\left(\frac{N}{V}\right)$ determine A

A increases when T decreases

$\left(\frac{N}{V}\right)$ increases.

But $F(B)$ cannot exceed 2.612

since B must > 1

In terms of relation

$$N = \underbrace{Z \cdot F(B)}$$

can only represent $2.612\,Z$ particles — may be less than N.

What has gone wrong?

Relation $N = \int_0^\infty g(k)\, f(k)\, dk$

assumes a smooth variation in population of states

At very low temperature - very large numbers of bosons go into ground state

Variation in population between ground state and excited states is not smooth.

Illustration — see sheet.

This excess population of ground state called Bose-Einstein Condensation. - occurs for temperatures T below a critical temp T_B.

Critical condition

$$B = 1 \qquad F(B) = 2.612$$

Then

$$2.612 = \left(\frac{N}{V}\right)\left(\frac{h^2}{2\pi m k T_B}\right)^{3/2}$$

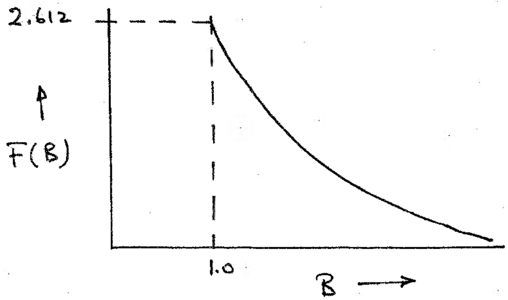
gives critical temp T_B as

$$T_B = \left(\frac{h^2}{2\pi m k}\right)\left(\frac{N}{2.612\ V}\right)^{2/3}$$

Bose - Einstein gas.

Graph of $F(B)$ vs B

where $$F(B) = \frac{4}{\sqrt{\pi}} \int_0^\infty \frac{y^2\,dy}{B\exp(y^2) - 1}$$



Points

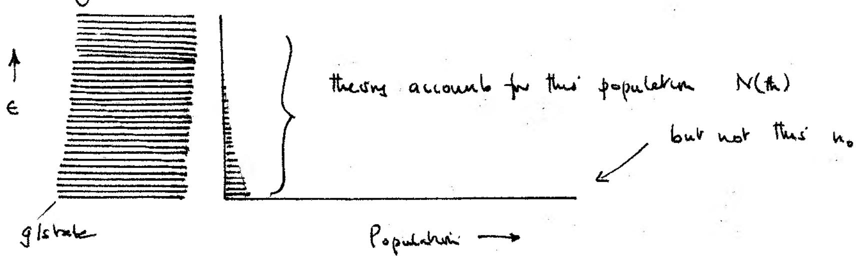
(i) For $B \gg 1$ $\quad F(B) \to \frac{1}{B}$

(ii) $F(B)$ only defined in range $1 < B$

(iii) For $B = 1$ $\quad F(B) = 2.612.$

Population of states by bosons at low temperature

Quantum states



110

Population in ground state

Total number particles = Number in ground state + Number in exited states

$$N = n_o + N(th)$$

Degeneracy of g/state $= g_o$

$$n_o = g_o \cdot \frac{1}{(B-1)}$$

$N(th)$ — given by distribution.

For temperatures $T > T_B$

No B-E condensation

$B > 1$

n_o — not large

$$N(th) = V\left(\frac{2\pi mkT}{h^2}\right)^{3/2} F(B).$$

For temperatures $T < T_B$

$$N(th) = Z \times 2.612 = 2.612\, V\left(\frac{2\pi mkT}{h^2}\right)^{3/2}$$